Some Discrete Tools in Statistical Physics

Martin Loebl¹

Charles University, Prague

Abstract. We will be walking for some time where the connections between combinatorics and statistical physics lead us.

Keywords. Graph, partition function, Ising problem, dimer arrangement, knot diagram

1. Beginning

The purpose of this note is to describe in passing some beautiful basic concepts interlacing statistical physics, combinatorics and knot theory. There are many sources and the time constraint prevented me from adding the references; this is just an informal writeup, anyway. If you get hooked up in a topic, your library will have more detailed books on the subject probably. I am also writing a book which should roughly cover the themes of this paper.

A graph is a pair (V, E) where V is a set of vertices and E is a set of unordered pairs from V, called *edges*. The notions of graph theory we will use are so natural there is no need to introduce them.

1.1. Euler's Theorem

Perhaps the first theorem of graph theory is the Euler's theorem, and it is also about walking.

THEOREM 1 A graph G = (V, E) has a closed walk containing each edge exactly once if and only if it is connected and each vertex has an even number of edges incident with it.

This theorem has an easy proof. Let us call a set A of edges *even* if each vertex of V is incident with an even number of edges of A. Connectivity and evenness are clearly necessary conditions for the existence of such a closed walk. Sufficiency follows from the following two lemmas.

LEMMA 1 Each even set of edges is a disjoint union of sets of edges of cycles.

¹Correspondence to: Martin Loebl, Dept. of Applied Mathematics and Institute of Theoretical Computer Science (ITI), Charles University, Malostranske n. 25, 118 00 Praha 1, Czech Republic; E-mail: loebl@kam.mff.cuni.cz

LEMMA 2 A connected set of disjoint cycles admits a closed walk which goes through each edge exactly once.

The first lemma might be called *the greedy principle of walking*: to prove the first lemma we observe first that each non-empty even set contains a cycle; if we delete it, we again get an even set and we can continue in this way until the remaining set is empty. The proof of the second lemma is also simple: we can compose the closed walk by the walks along the disjoint cycles.

1.2. Even sets of edges as a kernel

We will often not distinguish a subset A of edges and its incidence vector χ_A , i.e. 0, 1-vector indexed by the edges of G, with $(\chi_A)_e = 1$ iff $e \in A$. Let $\mathcal{E}(G)$ be the set of the even subsets of edges of the graph G.

We denote by I_G the *incidence matrix* of graph G, i.e. matrix with rows indexed by V(G), columns indexed by E(G), and $(I_G)_{ve}$ equal to one if $v \in e$ and zero otherwise. We immediately have

Observation 1 $\mathcal{E}(G)$ forms the GF[2]-kernel of I_G , i.e. $\mathcal{E}(G) = \{v; I_G v = 0 \text{ modulo } 2\}$.

What is the orthogonal complement of $\mathcal{E}(G)$ in $GF[2]^{E(G)}$? It is the set $\mathcal{C}(G)$ of edge-cuts of G; a set A of edges is called *edge-cut* if there is a set U of vertices such that $A = \{e \in E; |e \cap U| = 1\}.$

1.3. Max-Cut, Min-Cut problems

Max-Cut and Min-Cut problems belong to the basic hard problems of computer science. Given a graph G = (V, E) with a (rational) weight w(e) assigned to each edge $e \in E$, the Max-Cut problem asks for the maximum value of $\sum_{e \in C} w(e)$ over all edge-cuts of G, while the Min-Cut problem asks for the minimum of the same function.

Max-Cut problem is hard (NP-complete) for non-negative edge-weights and hence both Max-Cut and Min-Cut problems are hard for general rational edge-weights. The Min-Cut problem is efficiently (polynomially) solvable for non-negative edge-weights. This has been a fundamental result of computer science, and is known as 'max-flow, min-cut algorithm'.

Still, there are some special important classes of graphs where the Max-Cut problem is efficiently solvable. One such class is the class of the planar graphs.

1.4. Max-Cut problem for planar graphs

A graph is called *planar* if it can be represented in the plane so that the vertices are different points, the edges are *arcs* (by arc we mean an injective continuous map of the closed interval [0, 1] to the plane) connecting the representations of their vertices, and disjoint with the rest of the representation. We will also say that the planar graphs have *proper planar drawing*, and a properly drawn planar graph will be called *topological planar graph*. Let G be a topological planar graph and let γ be the subset of the plane consisting of the plane representation of G. After deletion of γ , the plane is partitioned

into 'islands' which are called *faces* of G. We let F(G) be the set of the faces of G and we will denote by v(G), e(G), f(G) the number of vertices, edges and faces of G and recall the Euler's formula: v(G) - e(G) + f(G) = 2.

An important concept we need is that of *dual graph* G^* of a topological graph G. It turns out convenient to define G^* as an abstract (not topological) graph. But we need to allow multiple edges and loops which is not included in the concept of the graph as a pair (V, E), where $E \subset {V \choose 2}$.

A standard way out is to define a graph as a triple (V, E, g) where V, E are sets and g is a function from E to $\binom{V}{2} \cup V$ which gives to each edge its terminal vertices. For instance $e \in E$ is a loop iff $g(e) \in V$.

Now we can define G^* as triple $(F(G), \{e^*; e \in E(G)\}, g)$ where $g(e^*) = \{f \in F(G); e \text{ belongs to the boundary of } f\}$.

If G is a topological planar graph then G^* is planar. There is a natural way to properly draw G^* to the plane: represent each vertex $f \in F(G)$ as a point in the face f, and represent each edge e^* by an arc between the corresponding points, which crosses exactly once the representation of e in G and is disjoint with the rest of the representations of G and G^* .

We will say that a set A of edges of a topological planar graph is dual even if $\{e^*; e \in A\}$ is an even set of edges of G^* .

Observation 2 The dual even subsets of edges of G are exactly the edge-cuts of G^* .

These considerations reduce the Max-Cut problem in the class of the planar graphs to the following problem, again in the class of the planar graphs:

Maximum even subset problem. Given a graph G = (V, E) with rational weights on the edges, find the maximum value of $\sum_{e \in H} w(e)$ over all even subsets H of edges.

Finally the following theorem means that the Max-Cut problem is efficiently solvable for the planar graphs.

THEOREM 2 The Maximum even subset problem is efficiently solvable for general graphs.

1.5. Edwards-Anderson Ising model

The Max-Cut problem has a long history in computer science, but one of the basic applications comes from the study of the *Ising model*, a theoretical physics model of the nearest-neighbor interactions in a crystal structure.

In the Ising model, the vertices of a graph G = (V, E) represent particles and the edges describe interactions between pairs of particles. The most common example is a planar square lattice where each particle interacts only with its neighbors. Often, one adds edges connecting the first and last vertex in each row and column, which represent *periodic boundary conditions* in the model. This makes the graph a *toroidal square lattice*.

Now, we assign a factor J_{ij} to each edge $\{i, j\}$; this factor describes the nature of the interaction between particles *i* and *j*. A physical state of the system is an assignment of $\sigma_i \in \{+1, -1\}$ to each vertex *i*. This describes the two possible spin orientations the particle can take. The *Hamiltonian* (or *energy function*) of the system is then defined as

Martin Loebl / Some Discrete Tools in Statistical Physics

$$H(\sigma) = -\sum_{\{i,j\}\in E} J_{ij}\sigma_i\sigma_j$$

One of the key questions we may ask about a specific system is:

"What is the lowest possible energy (the ground state) of the system?"

Before we seek an answer to this question, we should realize that the physical states (spin assignments) correspond exactly to the edge-cuts of the underlying graph with specified 'shores'. Let us define:

$$V_1 = \{i \in V; \sigma_i = +1\}$$

$$V_2 = \{i \in V; \sigma_i = -1\}$$

Then this partition of vertices encodes uniquely the assignment of spins to particles. The edges contained in the edge-cut $C(V_1, V_2)$ are those connecting a pair of particles with different spins, and those outside the cut connect pairs with equal spins. This allows us to rewrite the Hamiltonian in the following way:

$$H(\sigma) = \sum_{\{i,j\} \in C} J_{ij} - \sum_{\{i,j\} \in E \setminus C} J_{ij} = 2w(C) - W_{j}$$

where $w(C) = \sum_{\{i,j\} \in C} J_{ij}$ denotes the weight of a cut, and $W = \sum_{\{i,j\} \in E} J_{ij}$ is the sum of all edge weights in the graph.

Clearly, if we find the value of MAX-CUT, we have found the maximum energy of the physical system. Similarly, MIN-CUT (the cut with minimum possible weight) corresponds to the minimum energy of the system.

The distribution of the physical states over all possible energy levels is encapsulated in the *partition function*:

$$Z(G,\beta) = \sum_{\sigma} e^{-\beta H(\sigma)}.$$

The variable β is changed for K/T in the Ising model, where K is a constant and T is a variable representing the temperature.

It follows from 1.4 that there is an efficient algorithm to determine the ground state energy of the Ising model on any planar graph. In fact the whole partition function may be determined efficiently for planar graphs, and a principal ingredient is the following concept of 'enumeration duality'.

4

1.6. An enumeration duality

It turns out that the Ising partition function for a graph G may be expressed in terms of the generating function of the even sets of the same graph G. This is the seminal theorem of Van der Waerden whose proof is so simple that we include it here. We will use the following standard notations: $\sinh(x) = 1/2(e^x - e^{-x})$, $\cosh(x) = 1/2(e^x + e^{-x})$, $\tanh(x) = \frac{\sinh(x)}{\cosh(x)}$.

THEOREM **3** Let G = (V, E) be a graph with edge weights $J_{ij}, ij \in E$. Then

$$Z(G,\beta) = 2^{|V|} \prod_{ij \in E} \cosh(\beta J_{ij}) \mathcal{E}(G,x)|_{x^{J_{ij}} := \tanh(\beta J_{ij})}$$

Proof. We have

$$Z(G,\beta) = \sum_{\sigma} e^{\beta \sum_{ij} J_{ij}\sigma_i\sigma_j} = \sum_{\sigma} \prod_{ij\in E} (\cosh(\beta J_{ij}) + \sigma_i\sigma_j \sinh(\beta J_{ij})) =$$

$$\prod_{ij\in E} \cosh(\beta J_{ij}) \sum_{\sigma} \prod_{ij\in E} (1+\sigma_i \sigma_j \tanh(\beta J_{ij})) = \prod_{ij\in E} \cosh(\beta J_{ij}) \sum_{\sigma} \sum_{A\subset E} \prod_{ij\in E} \sigma_i \sigma_j \tanh(\beta J_{ij}) = \prod_{ij\in E} (1+\sigma_i \sigma_j \tanh(\beta J_{ij})) = \prod_{ij\in E} (1+\sigma_i m_i \prod(\beta J_{ij})) = \prod_{$$

$$\prod_{ij\in E} \cosh(\beta J_{ij}) \sum_{A\subset E} (U(A) \prod_{ij\in A} \tanh(\beta J_{ij})),$$

where

$$U(A) = \sum_{\sigma} \prod_{ij \in A} \sigma_i \sigma_j.$$

The proof is complete when we notice that $U(A) = 2^{|V|}$ if A is even and U(A) = 0 otherwise.

We saw above that $Z(G, \beta)$ may be looked at as the generating function of the edgecuts with the specified shores. The theorem of Van der Waerden expresses it in terms of the generating function $\mathcal{E}(G, x)$ of the even sets of edges.

We can also consider the honest generating function of edge-cuts defined by

$$\mathcal{C}(G, x) = \sum_{cutC} x^{w(C)},$$

where the sum is over all edge-cuts of G and $w(C) = \sum_{e \in C} w(e).$

It turns out that C(G, x) may also be expressed in terms of $\mathcal{E}(G, x)$. This is a consequence of another seminal theorem, of MacWilliams which we explain now.

Let $C \subset GF[2]^n$ be a *binary code*, i.e. a subspace over GF[2]. Let $A_i(C)$ denote the number of vectors of C with exactly i occurrences of 1. The *weight enumerator* of C is defined as

Martin Loebl / Some Discrete Tools in Statistical Physics

$$A_C(y) = \sum_{i \ge 0} A_i(C) y^i.$$

let us denote by C^* the *dual code*, i.e. the orthogonal complement of C. MacWilliam's theorem reads as follows:

THEOREM 4

$$A_{C^*}(y) = \frac{1}{|C|} (1+y)^n A_C(\frac{1-y}{1+y}).$$

We saw before that the set of the edge-cuts and the set of the even sets of edges form dual binary codes, hence MacWilliams' theorem applies.

This theorem is true more generally for linear codes over finite field GF[q]; hence it applies to the kernel and the image of the incidence matrix of a graph, viewed over GF[q]. This is related to the extensively studied field of *nowhere-zero flows*.

1.7. A game of dualities: critical temperature of 2D Ising model

We will end this introductory part by an exhibition of a game of dualities. We will assume that our graph G = (V, E) is a planar square grid, and we denote by N its number of vertices. This is a rude specialisation for the graph-theorists, but not for statistical physicists since planar square grids are of basic importance for 2-dimensional Ising problem. Moreover for simplicity we will have all the edges of the same weight, i.e. $J_{ij} = J$ for each $ij \in E$. Hence

$$Z(G,\beta) = Z(N,\gamma) = \sum_{\sigma} e^{\gamma \sum_{ij \in E} \sigma_i \sigma_j},$$

where $\gamma = J/T$ and T represents the temperature.

We will take advantage of the interplay between the geometric duality and the enumeration duality (Theorem 3). Let G^* denote the dual graph of G. A great property of the planar square grids is that they are essentially self-dual; on the boundary there are some differences, but who cares, we are playing anyway. So we will **cheat** and assume that $G = G^*$.

Low temperature expansion. Here we use the geometric duality. The states σ correspond to the assignments of + or - to the plaquettes of G^* . An edge of G^* will be called *frontal* for this assignment if it borders two plaquettes with the opposite signs. Now we observe that the set of the frontal edges for an assignment is even, and each even set of edges of G^* corresponds to exactly two states σ (which are opposite on each vertex). Summarising,

$$Z(N,\gamma) = 2e^{|E|\gamma} \sum_{H} e^{-2|H|\gamma},$$

where the sum is over all even subsets of edges of $G^* = G$.

If T goes to zero then γ goes to infinity, and hence small cycles should dominate this expression of the partition function. This is a good news for computer simulations, and explains the name of this formula.

6

High temperature expansion. Here we use Theorem 3. It honestly gives

$$Z(N,\gamma) = 2^N \cosh(\gamma)^{|E|} \sum_H \tanh(\gamma)^{|H|},$$

where the sum is again over all even subsets of edges of G.

If T goes to infinity then γ goes to zero, and hence small cycles should dominate this expression of the partition function.

Critical temperature of 2D Ising model. Let $F(\gamma)$ be the *free energy per site*, i.e.

$$-F(\gamma) = \lim_{N \to \infty} N^{-1} \ln Z(N, \gamma).$$

At a critical point the free energy is non-analytic, so F will be a non-analytic function of γ . Moreover we *assume* that there is only one critical point. Then the expressions above help us to locate it: Let

$$F'(v) = \lim_{N \to \infty} N^{-1} \ln(\sum_{H} v^{|H|}),$$

where the sum is over all even subsets $H \subset E(G)$. Let $v = \tanh(\gamma)$. Then

$$-F(\gamma) = 2\gamma + F'(e^{-2\gamma}) = \ln(2\cosh(\gamma)) + F'(v).$$

If we define γ^* by $\tanh(\gamma^*) = e^{-2\gamma}$, we get

$$F(\gamma^*) = 2\gamma + F(\gamma) - \ln(2\cosh(\gamma)).$$

If γ is large, γ^* is small. Hence the last equation relates the free energy at a low temperature to that at a high temperature. Hence, if there is only one critical value γ_c , then necessarily $\gamma_c = \gamma_c^*$ and this determines it.

1.8. $\Delta - Y$ transformation

Let us try to apply the same trick to the honeycomb lattice H_{2N} with 2N vertices. If we disregard the boundary irregularities, its geometric dual is the triangular lattice T_N with N vertices. If we apply the high temperature expansion to H_{2N} and the low temperature expansion to T_N , we get an expression of $Z(H_{2N}, \gamma)$ in terms of $Z(T_N, \gamma)$.

In order to extract the critical temperature, we need one more relation, and we will get it from the $\Delta - Y$ transformation. This is one of these magic seminal simple local operations. It consists in the exchange of a vertex l of degree 3 connected to independent vertices i, j, k (a Y), with three edges between vertices i, j, k which form Δ (a triangle).

We first note that H_{2N} is bipartite, i.e. its vertices may be uniquelly partitioned into two sets V_1, V_2 so that all the edges go between them.

The new trick is to apply the $\Delta - Y$ transformation to all the vertices of V_1 . The result is again the triangular lattice T_N . Now, if we want to transform $Z(H_{2N}, \gamma)$ into the Ising partition function of this new triangular lattice T_N , we get a system of equations for the coupling constants of T_N , which has a solution, and this suffices to extract the critical temperature for $Z(H_{2N}, \gamma)$.

This system of equations in the operator form is the famous *Yang-Baxter equation*. It defines the *Temperley-Lieb algebra* which has been used to introduce and study the *quantum knot invariants* like Jones polynomial, with close connections to the topological QFTs.

This connection between statistical physics, knot theory, QFT and combinatorics has kept the mathematicians and physicists busy for more than a decade.

So, look where we arrived at from the Euler's theorem. Next chapter starts with another principle, *of inclusion and exclusion*.

2. Inclusion and Exclusion

Let us start with the introduction of a paper of Hassler Whitney, which appeared in Annals of Mathematics in August 1932:

"Suppose we have a finite set of objects (for instance books on a table), each of which either has or has not a certain given property A (say of being red). Let n be the total number of objects, n(A) the number with the property A, and $n(\bar{A})$ the number without the property A. Then obviously $n(\bar{A}) = n - n(A)$. Similarly, if n(AB) denote the number with both properties A and B, nad $n(\bar{A}\bar{B})$ the number with neither property, then $n(\bar{A}\bar{B}) = n - n(A) - n(B) + n(AB)$, which is easily seen to be true.

The extension of these formulas to the general case where any number of properties are considered is quite simple, and is well known to logicians. It should be better known to mathematicians also; we give in this paper several applications which show its usefulness."

Indeed, we all know it, under the name 'inclusion-exclusion principle': if $A_1, ..., A_n$ are finite sets, and if we let $\bigcap (A_i; i \in J) = A_J$ then

$$\left|\bigcup(A_i; i=1, ..., n)\right| = \sum_{k=1}^n (-1)^{k-1} \sum_{J \in \binom{n}{k}} |A_J|.$$

It can also be formulated as follows:

THEOREM 5 Let S be an n-element set and let V be a 2^n -dimensional vector space over some field K. We consider the vectors of V indexed by the subsets of S. Let l be a linear transformation on V defined by

$$l(v_T) = \sum_{T \subset Y} v_Y$$

for all $T \subset S$. Then l^{-1} exists and is given by

$$l^{-1}(v_T) = \sum_{T \subset Y} (-1)^{|Y-T|} v_Y$$

for all $T \subset S$.

The set of all subsets of S equipped with the relation ' \subset ' forms a partially ordered set (poset) called *Boolean poset*. The *Mobius inversion formula* extends Theorem 5 from the Boolean poset to an arbitrary 'locally finite' poset.

2.1. Zeta Function of a Graph

The theory of the Mobius function connects the Principle of Inclusion and Exclusion with a very useful concept of the *zeta function of a graph*. We will explain a seminal theorem of Bass. You will see in the last section of the paper that it is closely related to (several decades older) combinatorial solution to the 2D Ising model proposed by Kac, Ward and Feynman.

Let G = (V, E) be a graph and let A = (V, A(G)) be an arbitrary orientation of G; an *orientation* of a graph is a prescribtion of one of two *directions* to each edge. If $e \in E$ then a_e will denote the orientation of e in A(G) and a_e^{-1} will be the reversed orientation to a_e . A 'circular sequence' $p = v_1, a_1, v_2, a_2, ..., a_n, (v_{n+1} = v_1)$ is called *prime reduced cycle* if the following conditions are satisfied: $a_i \in \{a_e, a_e^{-1} : e \in E\}$, $a_i \neq a_{i+1}^{-1}$ and $(a_1, ..., a_n) \neq Z^m$ for some sequence Z and m > 1.

DEFINITION 1 Let G = (V, E) be a graph. The Ihara-Selberg function of G is

$$I(u) = \prod_{\gamma} (1 - u^{|\gamma|})$$

and the zeta function of G is

$$Z(u) = I(u)^{-1},$$

where the infinite product is over the set of the prime reduced cycles γ of G.

The theorem of Bass reads as follows:

THEOREM 6

$$I(u) = \det(I - uT),$$

where T is the matrix of the transitions between edges.

The above considerations are closely related to the MacMahon's Master Theorem, known also as *boson-fermion correspondence* in physics. Strong connections with quantum knot invariants have been discovered recently.

THEOREM 7 The coefficient of $x_1^{m_1} \dots x_n^{m_n}$ in

$$\prod_{i=1}^{n} (\sum_{j=1}^{n} a_{ij} x_j)^{m_i}$$

is equal to the coefficient of $z_1^{m_1} \dots z_n^{m_n}$ in the power series expansion of $[\det(\delta_{ij} - a_{ij}z_i)]^{-1}$.

3. The chromatic polynomial and the Tutte polynomial

In the before-mentioned paper, Whitney mentions a formula for the number of ways of coloring a graph as one of the main applications of PIE. Let us again follow the article of Whitney for a while:

Suppose we have a fixed number z of colors at our disposal. Any way of assigning one of these colors to each vertex of the graph in such a way that any two vertices which are joined by an arc are of different colors, will be called admissible coloring, using z or fewer colors. We wish to find the number M(z) of admissible colorings, using z or fewer colors. ... We shall deduce a formula for M(z) due to Birkhoff.

If there are V vertices in the graph G, then there are $n = z^V$ possible colorings, formed by giving each vertex in succession any one of z colors. Let R be this set of colorings. Let A_{ab} denote those colorings with the property that a and b are of the same color, etc. Then the number of admissible colorings is

$$M(z) = n - [n(A_{ab}) + n(A_{bd}) + \dots + n(A_{cf})] + [n(A_{ab}A_{bd}) + \dots] - \dots + (-1)^E n(A_{ab}A_{bd} \dots A_{cf}).$$

With each property A_{ab} is associated an arc ab of G. In the logical expansion, there is a term corresponding to every possible combination of the properties A_{pq} ; with this combination we associate the corresponding edges, forming a subgraph H of G. In particular, the first term corresponds to the subgraph containing no edges, and the last term corresponds to the whole of G. We let H contain all the vertices of G.

Let us evaluate a typical term $n(A_{ab}A_{ad}...A_{ce})$. This is the number of ways of coloring G in z or fewer colors in such a way that a and b are of the same color, a and d are of the same color, ..., c and e are of the same color. In the corresponding subgraph H, any two vertices that are joined by an edge must be of the same color, and thus all the vertices in a single connected piece in H are of the same color. If there are p connected pieces in H, the value of this term is therefore z^p . If there are s edges in H, the sign of the term is $(-1)^s$. Thus

$$(-1)^{s} n(A_{ab}A_{bd}...A_{cf}) = (-1)^{s} z^{p}.$$

If there are (p, s) (this is Birkhoff's symbol) subgraphs of s edges in p connected pieces, the corresponding terms contribute to M(z) an amount $(-1)^s(p, s)z^p$. Therefore, summing over all values of p and s, we find the polynomial in z:

$$M(z) = \sum_{p,s} (-1)^s (p,s) z^p.$$

This function is the well-known *chromatic polynomial*. The proper colorings of graphs appeared perhaps first with the famous Four-Color-Conjecture, which is now a

theorem, even though proved only with a help of computers: Is it true that each planar graph has an admissible coloring by four colors?

A graph G = (V, E) is *connected* if it has a path between any pair of vertices. If a graph is not connected then its maximum connected subgraphs are called *connected components*. If G = (V, E) is a graph and $A \subset E$ then let C(A) denote the set of the connected components of graph (V, A) and c(A) = |C(A)| denotes the number of connected components (pieces) of (V, A).

Let G = (V, E) be a graph. For $A \subset E$ let r(A) = |V| - c(A). Then we can write

$$M(z) = z^{c(E)} (-1)^{r(E)} \sum_{A \subset E} (-z)^{r(E) - r(A)} (-1)^{|A| - r(A)}.$$

This leads directly to Whitney rank generating function R(G, u, v) defined by

$$R(G, u, v) = \sum_{A \subset E} u^{r(E) - r(A)} v^{|A| - r(A)}.$$

We start considering the *Tutte polynomial*; it has been defined by Tutte and it may be expressed as a minor modification of the Whitney rank generating function.

$$T(G, x, y) = \sum_{A \subset E} (x - 1)^{r(E) - r(A)} (y - 1)^{|A| - r(A)}$$

T(G, x, y) is called the *Tutte polynomial* of graph G.

Note that for any connected graph G, T(G, 1, 1) counts the number of spanning trees of G: indeed, the only terms that count are those for which r(A) = r(E) = |A|. These are exactly the spanning trees of G.

The Tutte polynomial is directly related to the partition function of another basic model of statistical physics, the *Potts model*. Potts specialises to Ising.

3.1. The dichromate and the Potts partition function

The following function called *dichromate* is extensively studied in combinatorics. It is equivalent to the Tutte polynomial.

$$B(G, a, b) = \sum_{A \subset E} a^{|A|} b^{c(A)}.$$

DEFINITION 2 Let G = (V, E) be a graph, $k \ge 1$ integer and J_e a weight (coupling constant) associated with edge $e \in E$. The Potts model partition function is defined as

$$P^k(G, J_e) = \sum_s e^{E(P^k)(s)},$$

where the sum is over all functions (states) s from V to $\{1, \ldots, k\}$ and

$$E(P^k)(s) = \sum_{\{i,j\} \in E} J_{ij}\delta(s(i), s(j)).$$

We may write

$$P^{k}(G, J_{e}) = \sum_{s} \prod_{\{i,j\} \in E} (1 + v_{ij}\delta(s(i), s(j))) = \sum_{A \subset E} k^{c(A)} \prod_{\{i,j\} \in A} v_{ij},$$

where $v_{ij} = e^{J_{ij}} - 1$. The RHS is sometimes called *multivariate Tutte polynomial*; If all J_{ij} are the same we get an expression of the Potts partition function in the form of the dichromate:

$$P^{k}(G,x) = \sum_{s} \prod_{\{i,j\} \in E} e^{x\delta(s(i),s(j))} = \sum_{A \subset E} k^{c(A)}(e^{x}-1)^{|A|} = B(G,e^{x}-1,k)$$

3.2. The q-chromatic function and the q-dichromate

Here we study the following *q*-chromatic function on graphs:

DEFINITION **3** Let G = (V, E) be a graph and n a positive integer. Let $V = \{1, ..., k\}$ and let V(G, n) denote the set of all vectors $(v_1, ..., v_k)$ such that $0 \le v_i \le n - 1$ for each $i \le k$ and $v_i \ne v_j$ whenever $\{i, j\}$ is an edge of G. We define the q-chromatic function by:

$$M_q(G,n) = \sum_{(v_1 \dots v_k) \in V(G,n)} q^{\sum_i v_i}.$$

Note that $M_q(G, n)|_{q=1}$ is the classic chromatic polynomial of G. An example.

We first recall some notation:

For n > 0 let $(n)_1 = n$ and for $q \neq 1$ let $(n)_q = \frac{q^n - 1}{q - 1}$ denote a *quantum integer*. We let $(n)!_q = \prod_{i=1}^n (i)_q$ and for $0 \le k \le n$ we define the *quantum binomial coefficients* by

$$\binom{n}{k}_q = \frac{(n)!_q}{(k)!_q(n-k)!_q}.$$

A simple quantum binomial formula leads to a well-known formula for the summation of the products of distinct powers. This gives the q-chromatic function for the complete graph.

Observation 3

$$M_q(K_k, n) = k! \binom{n}{k}_q q^{k(k-1)/2}.$$

Let G = (V, E) be a graph and $A \subset E$ with C(A) denoting the set of the connected components of graph (V, A) and c(A) = |C(A)|. If $W \in C(A)$ then let |W| denote the number of vertices of W. A standard PIE argument gives the following expression for the q-chromatic function, which enables to extend it from non-negative n to the reals.

THEOREM 8

$$M_q(G,n) = \sum_{A \subset E} (-1)^{|A|} \prod_{W \in C(A)} (n)_{q^{|W|}}.$$

The formula of Theorem 8 leads naturally to a definition of *q*-dichromate.

DEFINITION 4 We let

$$B_q(G, x, y) = \sum_{A \subset E} x^{|A|} \prod_{W \in C(A)} (y)_{q^{|W|}}$$

Note that $B_{q=1}(G, x, y) = B(G, x, y)$ and by Theorem 8, $M_q(G, n) = B_q(G, -1, n)$. What happens if we replace $B(G, e^x - 1, k)$ by $B_q(G, e^x - 1, k)$? It turns out that this introduces an additional external field to the Potts model.

THEOREM 9

$$\sum_{A \subset E} \prod_{W \in C(A)} (k)_{q^{|W|}} \prod_{\{i,j\} \in A} v_{ij} = \sum_{s} q^{\sum_{v \in V} s(v)} e^{E(P^k)(s)},$$

where $v_{ij} = e^{J_{ij}} - 1$.

3.3. Multivariate generalisations

Let x_1, x_2, \ldots be commuting indeterminates and let G = (V, E) be a graph. The qchromatic function restricted to non-negative integer y is the principal specialization of X_G , the symmetric function generalisation of the chromatic polynomial. This has been defined by Stanley as follows:

DEFINITION 5

$$X_G = \sum_f \prod_{v \in V} x_{f(v)},$$

where the sum ranges over all proper colorings of G by $\{1, 2, ...\}$.

Therefore $M_q(G, n) = X_G(x_i = q^i (0 \le i \le n - 1), x_i = 0 (i \ge n))$. Further Stanley defines symmetric function generalisation of the bad colouring polynomial:

DEFINITION 6

$$XB_G(t, x_1, \dots) = \sum_{f} (1+t)^{b(f)} \prod_{v \in V} x_{f(v)},$$

where the sum ranges over ALL colorings of G by $\{1, 2, ...\}$ and b(f) denotes the number of monochromatic edges of f.

Noble and Welsh define the *U-polynomial* (see Definition 7) and show that it is equivalent to XB_G . Sarmiento proved that the polychromate defined by Brylawski is also equivalent to the U-polynomial.

DEFINITION 7

$$U_G(z, x_1...) = \sum_{S \subseteq E(G)} x(\tau_S)(z-1)^{|S|-r(S)}$$

where $\tau_S = (n_1 \ge n_2 \ge \dots n_k)$ is the partition of |V| determined by the connected components of S, $x(\tau_S) = x_{n_1} \dots x_{n_k}$ and r(S) = |V| - c(S).

The motivation for the work of Noble and Welsh is a series of papers by Chmutov, Duzhin and Lando. It turns out that the U-polynomial evaluated at z = 0 and applied to the intersection graphs of chord diagrams satisfies the 4T-relation of the *weight systems*. Hence the same is true for $M_q(G, z)$ for each positive integer z since it is an evaluation of $U_G(0, x_1 \dots)$:

Observation 4 Let z be a positive integer. Then

$$M_q(G,z) = (-1)^{|V|} U_G(0,x_1\dots)|_{x_i:=(-1)(q^{i(z-1)}+\dots+1)}.$$

1 7 7 1

Weight systems form a basic stone in the combinatorial study of the quantum knot invariants.

On the other hand, it seems plausible that the q-dichromate determines the Upolynomial. If true, q-dichromate provides a compact representation of the multivariate generalisations of the Tutte polynomial mentioned above.

4. Two combinatorial solutions to the 2D Ising model

In this section we describe two ways how to calculate the partition function of the Ising model for any given planar graph G. We have seen in Theorem 3 that the Ising partition function for graph G may be calculated from the generating function $\mathcal{E}(G, x)$ of the even subsets of edges of the same graph G.

4.1. The method of Pfaffian orientations

Let G = (V, E) be a graph. A subset of edges $P \subset E$ is called a *perfect matching* or *dimer arrangement* if each vertex belongs to exactly one element of P. The *dimer partition function* on graph G may be viewed as a polynomial $\mathcal{P}(G, \alpha)$ which equals the sum of $\alpha^{w(P)}$ over all perfect matchings P of G. This polynomial is also called the *generating function of perfect matchings*. There is a simple local transformation of graph

G to graph *G'* so that $\mathcal{E}(G) = \mathcal{P}(G')$, and *G'* is planar if *G* is. Hence in order to calculate $\mathcal{E}(G)$, it suffices to show how to calculate $\mathcal{P}(G)$ for the planar graphs *G*.

An orientation of a graph G = (V, E) is a *digraph* D = (V, A) obtained from G by assigning an orientation to each edge of G, i.e. by ordering the elements of each edge of G.

Let G = (V, E) be a graph with 2n vertices and D an orientation of G. Denote by A(D) the skew-symmetric matrix with the rows and the columns indexed by V, where $a_{uv} = \alpha^{w(u,v)}$ in case (u, v) is a directed edge of D, $a_{u,v} = -\alpha^{w(u,v)}$ in case (v, u) is a directed edge of D, and $a_{u,v} = 0$ otherwise.

DEFINITION 8 The Pfaffian is defined as

$$Pf_G(D,\alpha) = \sum_P s^*(P)a_{i_1j_1}\cdots a_{i_nj_n},$$

where $P = \{\{i_1j_1\}, \dots, \{i_nj_n\}\}$ is a partition of the set $\{1, \dots, 2n\}$ into pairs, $i_k < j_k$ for $k = 1, \dots, n$, and $s^*(P)$ equals the sign of the permutation $i_1j_1 \dots i_nj_n$ of $12 \dots (2n)$.

Each nonzero term of the expansion of the Pfaffian equals $\alpha^{w(P)}$ or $-\alpha^{w(P)}$ where P is a perfect matching of G. If s(D, P) denotes the sign of the term $\alpha^{w(P)}$ in the expansion, we may write

$$Pf_G(D, \alpha) = \sum_P s(D, P)\alpha^{w(P)}.$$

The Pfaffians behave in a way very similar to determinants; in particular there is an efficient Gaussian elimination algorithm to calculate them.

Hence, if we can find, for a graph G, an orientation D such that the sign s(D, P) from 8 is the same for each perfect matching P, then we can calculate the generating function of the perfect matchings of G efficiently. Such an orientation is called *Pfaffian* orientation.

The following seminal theorem of Kasteleyn thus provides a solution of the 2D Ising problem.

THEOREM 10 Each planar graph has a Pfaffian orientation.

We can draw graphs on more complicated 2-dimensional surfaces; let us consider those that can be represented as the sphere with added disjoint handles (the torus is obtained from the sphere by adding one handle). The *genus* of a graph is the minimum number of handles needed for its proper representation. Kasteleyn noticed and Galluccio, Loebl proved the following generalisation of theorem 10.

THEOREM 11 If G is a graph of genus g then it has 4^g orientations D_1, \ldots, D_{4^g} so that $\mathcal{P}(G, x)$ is a linear combination of $Pf_G(D_i, x)$, $i = 1, \ldots, 4^g$.

As a consequence, the Ising partition function may be calculated in a polynomial time for graphs on any fixed orientable surface. Hence also the Max-Cut problem is polynomially solvable on any fixed surface, by exhibiting the whole density function of edgecuts weights. Curiously there is no other method known even for the torus. This brings a curious restriction to the weights: in order to write down the whole density function, the weights must be integers with the absolute values bounded by a fixed polynomial in the size of the graph. Perhaps the most interesting open problem in this area is to design a combinatorial polynomial algorithm for the toroidal Max-Cut problem.

4.2. Products over aperiodic closed walks

The following approach has been developed by Kac, Ward and Feynman. It coincides with the notions of 2.1. Let G = (V, E) be a planar graph embedded in the plane and for each edge e let x_e be an associate variable. Let A = (V, A(G)) be an arbitrary orientation of G. If $e \in E$ then a_e will denote the orientation of e in A(G) and a_e^{-1} will be the reversed orientation to a_e . We let $x_{a_e} = x_{a_e^{-1}} = x_e$. A circular sequence $p = v_1, a_1, v_2, a_2, ..., a_n, (v_{n+1} = v_1)$ is called *non-periodic closed walk* if the following conditions are satisfied: $a_i \in \{a_e, a_e^{-1} : e \in E\}$, $a_i \neq a_{i+1}^{-1}$ and $(a_1, ..., a_n) \neq Z^m$ for some sequence Z and m > 1. We let $X(p) = \prod_{i=1}^n x_{a_i}$. We further let $\operatorname{sign}(p) =$ $(-1)^{n(p)}$, where n(p) is a *rotation number* of p, i.e. the number of integral revolutions of the tangent vector. Finally let $W(p) = \operatorname{sign}(p)X(p)$.

There is a natural equivalence on non-periodic closed walks: p is equivalent with reversed p. Each equivalence class has two elements and will be denoted by [p]. We let W([p]) = W(p) and note that this definition is correct since equivalent walks have the same sign.

We denote by $\prod (1 - W([p]))$ the formal infinite product of (1 - W([p])) over all equivalence classes of non-periodic closed walks of G.

The following theorem, proposed by Feynman and proved by Sherman, together with a straightforward graph-theory transformation, provides an expression of $\mathcal{E}(G, x)^2$ for a planar graph G in terms of a reformulation of the Ihara-Selberg function of G by Foata and Zeilberger (see definition 1). The theorem thus provides, along with theorem 6, another solution of the 2D Ising problem. Again, there is a generalisation for graphs with genus g.

THEOREM 12 Let G be a planar graph with all degrees equal to two or four. Then

$$\mathcal{E}(G, x) = \prod (1 - W([p]))$$